# Equivalence of two definitions of the effective mass of a polaron

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Dedicated to Herbert Spohn, a leader in the mathematical study of the polaron, on the occasion of his retirement from T.U. München

#### Abstract

Two definitions of the effective mass of a particle interacting with a quantum field, such as a polaron, are considered and shown to be equal in models similar to the Fröhlich polaron model. These are: 1. the mass defined by the low momentum energy  $E(P) \approx E(0) + P^2/2M$  of the translation invariant system constrained to have momentum P and 2. the mass M of a simple particle in an arbitrary slowly varying external potential, V, described by the nonrelativistic Schrödinger equation, whose ground state energy equals that of the combined particle/field system in a bound state in the same V.

## 1 Introduction

When a particle, such as an electron, clothes itself with a quantized field of some kind, it is supposed to behave, to a good approximation, like a particle described by a different mass and, perhaps, a different charge. This

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belief notwithstanding, it has yet to be seen clearly, explicitly and nonperturbatively, how one can deduce the experimental Balmer lines of hydrogen from a fully interacting theory of quantum electrodynamics without cut-offs.

Herbert Spohn studied this question from a dynamical point of view [14, 17], showing that the dynamics of a dressed particle can be approximated to a certain extent by a simpler effective dynamics (see also [1, 15, 16]). This work is typical of his profound analysis of many fundamental aspects of theoretical physics. We study the same problem from a different, stationary, aspect, which is in some ways simpler and therefore might be of interest. We consider here the polaron model of H. Fröhlich [5], which describes an electron of bare mass m interacting with the quantized electric field of dipoles in a polar crystal; in contrast to quantum electrodynamics, there are no infinities in this theory that require renormalization. Spohn has pioneered much of the theoretical understanding of the polaron, especially its effective mass [4, 12, 13], and we hope these remarks may encourage him to continue his engagement with the subject.

The coupling constant in the model is denoted by  $\alpha$ . When  $\alpha$  is small perturbation theory does seem to be adequate, but usually  $\alpha$  is rather large. For very large  $\alpha$ , the approximate non-linear theory of Pekar [12] applies, at least to describe the ground state energy [2, 10]. The diameter of the polarization field cloud around the electron is proportional to  $\alpha^{-1}$  in Pekar's approximation.

We now place this object in a potential V that varies little over dimensions corresponding to the size of the cloud, and we ask the following question: Is it true that the ground state energy equals the polaron ground state energy, E(0), plus the non-relativistic Schrödinger ground state energy of a particle of mass M in the potential? Here, M is the effective mass of the polaron defined for the translation invariant problem (V=0) by the bottom of the spectrum in the momentum P fiber,  $E(P) \approx E(0) + P^2/2M$ , as  $P \to 0$ . In other words, can we define the effective, renormalized mass of a particle in two different, but equivalent ways: in terms of the ground state energy of the translation invariant problem (in the fiber of fixed total momentum P) or in terms of the ground state energy of the particle in a slowly varying potential well, such as an electron in the ground state of a hydrogen atom (as was attempted for nonrelativistic QED in [9])?

In this paper we show how this can be proved for the polaron, for any  $\alpha$ . Our method applies to a general class of models, as will be discussed after

Theorem 1 in the next section. Many open questions remain and some of these are reviewed at the end of the paper in Section 5.

### 2 Definition of the Problem and Main Result

The Hilbert space for a single polaron is

$$\mathcal{H} = L^2(\mathbb{R}^d) \otimes \mathcal{F}$$

where  $\mathcal{F}$  is the bosonic Fock space over  $L^2(\mathbb{R}^d)$ . Physically, it represents the electric field produced by the creation of dipoles in the optical mode of a polar crystal.

The Hamiltonian of the polaron is

$$H = p_x^2 + H_f + \int_{\mathbb{R}^d} v(k)e^{-ikx}a_k^{\dagger}dk + \int_{\mathbb{R}^d} \overline{v(k)}e^{ikx}a_kdk, \tag{1}$$

with  $p_x = -i\nabla_x$  (in units in which  $\hbar = 1$  and the particle mass equals m = 1/2), and with field energy

$$H_f = \int_{\mathbb{R}^d} \omega(k) a_k^{\dagger} a_k dk.$$

The momentum of a mode is denoted by  $k \in \mathbb{R}^d$ . For Fröhlich's polaron, d=3 and the energy of a mode,  $\omega(k)$ , is a positive constant, independent of k. Moreover, the interaction  $v(k) \propto \sqrt{\alpha} |k|^{-1}$  in this model. For our purposes here, however, we can consider general dimensions d as well as more general functions  $\omega(k)$  and v(k). We only require, at this point, that H defines a self-adjoint operator that is semi-bounded from below.

The important thing is that H commutes with total momentum  $\mathcal{P} = p_x + P_f$ , where  $P_f = \int_{\mathbb{R}^d} k a_k^{\dagger} a_k dk$ . There is the well known fiber decomposition in which H is restricted to states of a fixed numerical value, P, of  $\mathcal{P}$ , namely

$$H_P = (P - P_f)^2 + H_f + \int_{\mathbb{D}^d} v(k) a_k^{\dagger} dk + \int_{\mathbb{D}^d} \overline{v(k)} a_k dk, \tag{2}$$

which acts on  $\mathcal{F}$  alone. Then

$$H \cong \int_{\mathbb{R}^d}^{\oplus} H_P \, dP \, .$$

Define

$$E(P) = \inf \operatorname{spec} H_P$$
,

and define the "dynamic effective mass" M, which is greater than m = 1/2, by

$$\frac{1}{M} = 2 \lim_{P \to 0} \frac{E(P) - E(0)}{|P|^2}.$$
 (3)

We assume that this limit exists, but M need not be finite, a priori. For Fröhlich's polaron it is known that  $1/2 < M < \infty$  for all  $\alpha > 0$  [6, 8], i.e., there is no self-trapping of the electron.

To define the "static effective mass" M we let V be a bounded, real-valued function that decays at infinity and has the property that  $p_x^2 + V(x)$  has a negative energy bound state. (For technical reasons, we assume slightly more regularity, namely that the Fourier transform  $\hat{V}$  is in  $L^1(\mathbb{R}^d)$ .) Then the function

$$\mathcal{E}: [1/2, \infty) \to (-\infty, 0)$$
 ,  $\mathcal{E}(m) = \inf \operatorname{spec}\left(\frac{p_x^2}{2m} + V(x)\right)$ 

is negative and strictly decreasing for  $m \geq 1/2$ , and hence is invertible.

Note that, by scaling,  $p_x^2/2m + \lambda^2 V(\lambda x)$  for  $\lambda > 0$  is unitarily equivalent to  $\lambda^2(p_x^2/2m + V(x))$ . The definition of  $\widetilde{M}$  is

$$\mathcal{E}(\widetilde{M}) = \lim_{\lambda \to 0} \frac{1}{\lambda^2} \inf \operatorname{spec} \left( H + \lambda^2 V(\lambda x) - E(0) \right).$$

The purpose of  $\lambda$  here is merely to stretch the scale of V in order to insure that variations in V(x) have much longer wavelength than relevant modes of the field.

Our main result is the following.

**THEOREM 1.** Under suitable conditions on v and  $\omega$  (which are satisfied for Fröhlich's polaron model)

$$M = \widetilde{M} \tag{4}$$

To be precise, our theorem applies to all models of the form (1), satisfying the properties

(1) The limit (3) exists, and there is a constant C > 0 such that  $E(P) \ge E(0) + P^2[2M(1 + CP^2)]^{-1}$ 

(2) There exists a  $P_c > 0$  such that for all P with  $|P| < P_c$ ,  $H_P$  in (2) has a unique ground state, which depends continuously on P

These Assumptions are known to be fulfilled for the Fröhlich polaron, see [8] or [11]. Assumption (1) implies, in particular, that  $E(P) \geq E(0)$  for all  $P \in \mathbb{R}^d$ , and takes account of the fact that, in general, the function E(P) does not increase unboundedly. It is bounded above by  $\omega(P)$ , in fact. This is seen from (2) where we can obtain a variational upper bound to E(P) by using the state consisting of just one phonon of momentum k = P. Our proof of Theorem 1 is slightly complicated by the fact that we need to take account of the boundedness of E(P).

The proof of Theorem 1 consists of two steps. In Section 3, we shall show that Assumption (1) above implies that  $M \geq \widetilde{M}$ . The reverse inequality  $M \leq \widetilde{M}$  follows from Assumption (2) (and the first part of Assumption (1)), as shown in Section 4.

We remark that our method can be generalized to settings where Assumption (2) does not necessarily hold. For instance, for models of non-relativistic QED,  $\Phi_P$  does not exist for  $P \neq 0$  unless one introduces an infrared cut-off [6] (in addition to the necessary ultraviolet cut-off). One can either apply our method directly to a model with infrared cut-off, and then argue that the effective mass is continuous in the cut-off [7]. Alternatively, one could work with the full model (without infrared cutoff) but take as functions  $\Phi_P$  in our variation argument in Section 4 the ground states of the model with a suitable P-dependent cut-off. Given enough control of the dependence of these functions on P and the cut-off (as examined in [3] for the Nelson model for weak coupling) our argument applies.

3 
$$M \ge \widetilde{M}$$

With  $\mathcal{P} = p_x + P_f$  denoting the total momentum operator on  $\mathcal{H}$ , we have

$$H \geq E(\mathcal{P}).$$

This is so because, for each fiber, the number E(P) is the bottom of the spectrum. This function E is used to define the operator  $E(\mathcal{P})$ , which is unitarily equivalent to the operator  $E(p_x)$ , via the unitary transformation  $U = e^{ixP_f}$ . We note that  $U^*xU = x$ . Hence

inf spec 
$$(H + \lambda^2 V(\lambda x) - E(0)) \ge \inf \operatorname{spec} (E(p_x) + \lambda^2 V(\lambda x) - E(0))$$

and, therefore,

$$\mathcal{E}(\widetilde{M}) \ge \lim_{\lambda \to 0} \inf \operatorname{spec} \left( \frac{E(\lambda p_x) - E(0)}{\lambda^2} + V(x) \right),$$

where we applied a unitary rescaling of x by  $\lambda$ .

Let us assume that

$$E(P) \ge E(0) + \frac{P^2}{2M(1 + CP^2)} \tag{5}$$

for some C > 0. We claim that

inf spec 
$$\left(\frac{E(\lambda p_x) - E(0)}{\lambda^2} + V(x)\right) \ge \mathcal{E}(M) - O(\lambda)$$
 (6)

as  $\lambda \to 0$ , which implies that  $\mathcal{E}(\widetilde{M}) \geq \mathcal{E}(M)$ , hence  $M \geq \widetilde{M}$  since  $\mathcal{E}$  is a decreasing function.

For  $\beta > 0$ , let  $\chi(P) = \theta(\beta - |P|) = 1$  if  $|P| \le \beta$  and = 0 otherwise, and let  $\tilde{\chi}(P) = 1 - \chi(P)$ . From (5) we have

$$E(P) - E(0) \ge \chi(P) \frac{P^2}{2M(1 + C\beta^2)} + \tilde{\chi}(P) \frac{\beta^2}{2M(1 + C\beta^2)}.$$

We split  $V = V_+ - V_-$  into its positive and negative parts (i.e.,  $V_+(x) = \max\{V(x), 0\}$ ), and use Schwarz's inequality to bound  $\chi(\lambda p_x)V_\pm(x)\tilde{\chi}(\lambda p_x)$ . In this way we conclude that

$$V(x) \ge (1 - \epsilon)\chi(\lambda p_x)V_+(x)\chi(\lambda p_x) + (1 - \epsilon^{-1})\tilde{\chi}(\lambda p_x)V_+(x)\tilde{\chi}(\lambda p_x) - (1 + \epsilon)\chi(\lambda p_x)V_-(x)\chi(\lambda p_x) - (1 + \epsilon^{-1})\tilde{\chi}(\lambda p_x)V_-(x)\tilde{\chi}(\lambda p_x)$$

for any  $\epsilon > 0$ . We thus obtain

$$\frac{E(\lambda p_x) - E(0)}{\lambda^2} + V(x) 
\geq \chi(\lambda p_x) \left( \frac{p_x^2}{2M(1 + C\beta^2)} + (1 - \epsilon)V_+(x) - (1 + \epsilon)V_-(x) \right) \chi(\lambda p_x) 
+ \tilde{\chi}(\lambda p_x) \left( \frac{\beta^2}{2\lambda^2 M(1 + C\beta^2)} - (1 + \epsilon^{-1}) ||V||_{\infty} \right).$$

For the choice  $\epsilon = O(\lambda)$  and  $\beta = O(\lambda^{1/2})$ , one easily sees that

$$\frac{p_x^2}{2M(1+C\beta^2)} + (1-\epsilon)V_+(x) - (1+\epsilon)V_-(x) \ge \mathcal{E}(M) - O(\lambda).$$

Moreover, we can choose  $\epsilon = C\lambda$  with C large enough such that

$$\frac{\beta^2}{2\lambda^2 M (1 + C\beta^2)} - (1 + \epsilon^{-1}) ||V||_{\infty} \ge 0$$

for small  $\lambda$ . This gives the desired result (6).

4 
$$M \leq \widetilde{M}$$

Let  $\Phi_P \in \mathcal{F}$  denote the ground state of  $H_P$ , which we assume to exist and to be unique up to a phase for  $|P| < P_c$ . This is known to be the case for the Fröhlich polaron, see [8, Statement 1]. For  $x \in \mathbb{R}^d$ , let  $\Phi_P^x = \exp\{-ixP_f\}\Phi_P$ , and define  $\Psi \in \mathcal{H}$  as

$$\Psi = (2\pi\lambda)^{-d/2} \int_{\mathbb{R}^d} \hat{f}(\lambda^{-1}P) \exp\{iPx\} \Phi_P^x dP, \tag{7}$$

in which  $f \in L^2(\mathbb{R}^d)$  with ||f|| = 1 and  $\hat{f}$  is its Fourier transform (normalized so that  $||\hat{f}|| = 1$ ). We assume that  $\hat{f}$  has compact support, so that for small enough  $\lambda$  the integral in (7) is only over P's with  $|P| < P_c$ , where we know  $\Phi_P$  to exits. It is readily checked that  $||\Psi|| = 1$ . Moreover,

$$\langle \Psi | H \Psi \rangle = \int_{\mathbb{R}^d} |\hat{f}(P)|^2 E(\lambda P) dP$$

and

$$\langle \Psi | V(\lambda x) \Psi \rangle = (2\pi)^{-d/2} \int_{\mathbb{P}^{d} \times \mathbb{P}^{d}} \overline{\hat{f}(P)} f(P') \hat{V}(P - P') \langle \Phi_{\lambda P} | \Phi_{\lambda P'} \rangle dP dP',$$

where the latter inner product in the integrand is in  $\mathcal{F}$ . For fixed  $f \in H^1(\mathbb{R}^d)$ ,

$$\lim_{\lambda \to 0} \int_{\mathbb{R}^d} |\hat{f}(P)|^2 \frac{E(\lambda P) - E(0)}{\lambda^2} dP = \int_{\mathbb{R}^d} |\hat{f}(P)|^2 \frac{P^2}{2M} dP$$

by dominated convergence (using the fact that  $E(P) \leq E(0) + P^2$ ). If we now assume that  $\hat{V} \in L^1(\mathbb{R}^d)$ , we also have that

$$\lim_{\lambda \to 0} \int_{\mathbb{R}^d \times \mathbb{R}^d} \overline{\hat{f}(P)} f(P') \hat{V}(P - P') \langle \Phi_{\lambda P} | \Phi_{\lambda P'} \rangle dP dP'$$

$$= \int_{\mathbb{R}^d \times \mathbb{R}^d} \overline{\hat{f}(P)} f(P') \hat{V}(P - P') dP dP'.$$

Again we used dominated convergence, together with the continuity of  $\Phi_P$ , which implies that  $\langle \Phi_{\lambda P} | \Phi_{\lambda P'} \rangle$  converges to  $\langle \Phi_0 | \Phi_0 \rangle = 1$  as  $\lambda \to 0$ .

We have, therefore,

$$\mathcal{E}(\widetilde{M}) \le \lim_{\lambda \to 0} \left( \lambda^{-2} \langle \Psi | H - E(0) | \Psi \rangle + \langle \Psi | V(\lambda x) \Psi \rangle \right)$$

$$= \int_{\mathbb{R}^d} |\hat{f}(P)|^2 \frac{P^2}{2M} dP + \int_{\mathbb{R}^d} |f(x)|^2 V(x) dx \tag{8}$$

and this holds for any  $f \in L^2(\mathbb{R}^3)$  with  $\hat{f}$  having compact support. Taking the infimum over all such f's on the right side of (8) gives  $\mathcal{E}(M)$ , hence we indeed conclude that

$$\mathcal{E}(\widetilde{M}) \leq \mathcal{E}(M)$$
.

# 5 Outlook and Open Problems

The results reported here treat only the first of several related questions. Some of these will occur to the reader and some of them are stated here.

- Conjecture: Look at the ground state of  $H + \lambda^2 V(\lambda x)$  in  $\mathcal{H}$  for small  $\lambda$  and set  $x = y/\lambda$  with y fixed. This is a state in Fock space  $\mathcal{F}$ . When appropriately normalized, it should converge to  $\Phi_0$  (translated by x, i.e., conjugated with the unitary  $e^{ixP_f}$ ) as  $\lambda \to 0$ , irrespective of y.
- What is the relation of  $\Phi_0$  to Pekar's variational minimizer for the translation invariant problem when  $\alpha$  is large? We recall that this vector in  $\mathcal{H}$  is a simple tensor product of a vector  $\varphi$  in  $L^2(\mathbb{R}^3)$  and a vector (coherent state)  $\Phi_{\text{Pekar}} \in \mathcal{F}$ . Conjecture: For large  $\alpha$ , the ground state  $\Phi_0$  of  $H_P$  at P=0 is close to

$$\hat{\varphi}(P_f)\Phi_{\mathrm{Pekar}}$$

where  $P_f$  is the momentum operator on  $\mathcal{F}$  and  $\hat{\varphi}(P_f)$  is the Fourier transform of  $\varphi$ , as an operator on  $\mathcal{F}$ . On the level of n-phonon distributions this should be provable using the analysis in [10].

- An increase of  $\alpha$  can lead to a bound state of the system, even in the absence of any bound state for  $\alpha = 0$ . This "quantum phase transition" can be studied by our method, by introducing a potential V such that the operator  $p^2/(2m) + V(x)$  has a bound state only for  $m > m^* > 1/2$ . In order to study the precise dependence of this transition on V and  $\alpha$ , it is necessary to get quantitative bounds on the effective mass, which is a long-standing open problem.
- How can one describe the corrections to the identity (4) for small but non-zero  $\lambda$ ? These corrections lead to physically relevant effects, like the Lamb shift in quantum electrodynamics.

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